JOINT INSTITUTE FOR LABORATORY ASTROPHYSICS

UNIVERSITY OF COLORADO

REPORT

NATIONAL BUREAU OF STANDARDS

CLASSICAL PATH A AND B FUNCTIONS

FOR LINE BROADENING OF POSITIVE IONS

by

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JILA REPORT No. 105

University of Colorado

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NOTICE

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Abstract

The A, a and B functions for electron broadening of positive ions, that is, with an attractive hyperbolic path, are considered in detail for the dipole interaction. Functions for a repulsive hyperbola and quadrupole interactions are also discussed.

I. Introduction

When classical path calculations for impact broadening are performed a common procedure is to expand the required S-matrix elements to second order[1][2] and to express them in terms of A and B functions. In addition, when considering broadening of positive ions by electrons and ions, the classical trajectory is a hyperbola. In this report we consider the functions corresponding to dipole interactions of electrons in detail. Dipole interactions of ions and quadrupole interactions are also mentioned.

For an attractive potential (electron broadening)[3] the functions for a dipole interaction are

$$A(\xi,\varepsilon) + iB(\xi,\varepsilon)$$

$$= \frac{\varepsilon^2}{2}\int_{-\infty}^{\infty}dx\int_{-\infty}^{x}dy\frac{[\varepsilon^2+(\varepsilon^2-1)\mathrm{sh}x\,\mathrm{sh}y+\mathrm{ch}x\,\mathrm{ch}y-\varepsilon(\mathrm{ch}x+\mathrm{ch}y)]}{(\varepsilon\,\mathrm{ch}x-1)^2(\varepsilon\,\mathrm{ch}y-1)^2}e^{i\xi[\varepsilon(\mathrm{sh}x-\mathrm{sh}y)-(x-y)]} \quad . \quad (1)$$

For a particle of velocity v and impact parameter ρ causing a dipole transition between levels spaced ΔE apart of an ion of charge Z

$$\left.\begin{aligned} &\varepsilon = \sqrt{1+(\rho^2/a^2)} \;, \quad a = Ze^2/mv^2 \\ &\xi = Za\Delta E/\hbar v \end{aligned}\right\} \quad (2)$$

(notice ξ and ε are unsymmetrized in equation (2)).

The real part of equation (1) can be written in terms of modified Bessel functions[3][4]

$$A(\xi,\varepsilon) = (\xi\varepsilon)^2 e^{\pi\xi}[|K'_{i\xi}(\xi\varepsilon)|^2 + \frac{(\varepsilon^2-1)}{\varepsilon^2}|K_{i\xi}(\xi\varepsilon)|^2] \quad . \quad (3)$$

The imaginary part cannot be simply expressed and is calculated from the real part by means of the Hilbert transform

$$B(\xi,\varepsilon) = \frac{1}{\pi}\int_{0+}^{\infty} \frac{A(|\xi-x|,\varepsilon) - A(\xi+x,\varepsilon)}{x}\,dx \quad . \tag{4}$$

After the work described in this report was completed, fairly simple integral representations for the A and B functions have been found by S. Klarsfeld.[5] Our numerical results agree closely with his B function. For completeness, his results are

$$A(\xi,\varepsilon) = 4\xi^2\varepsilon^2 e^{\pi\xi}\int_0^{\infty} dt\, \cos\,(2\xi t)\mathrm{ch}^2 t\; K_0(2\xi\varepsilon\,\mathrm{ch}t)$$

$$B(\xi,\varepsilon) = 4\xi^2\varepsilon^2\int_0^{\pi/2} d\theta e^{2\xi\theta}\sin^2\theta\; K_0(2\xi\varepsilon\sin\theta)$$

$$- 4\xi^2\varepsilon^2 e^{\pi\xi}\int_0^{\infty} dt\, \sin(2\xi t)\mathrm{ch}^2 t\; K_0(2\xi\mathrm{ch}t) \quad .$$

To find the line-width it is also required to integrate the A function over impact parameters, to obtain

$$a(\xi,\varepsilon) = \int_{\varepsilon}^{\infty} A(\xi,\varepsilon')\,\frac{d\varepsilon'}{\varepsilon'} \tag{5}$$

$$= -e^{\pi\xi}(\xi\varepsilon)K'_{i\xi}(\xi\varepsilon)K_{i\xi}(\xi\varepsilon)$$

$$\left(= \xi\varepsilon^2 e^{\pi\xi}\int_0^{\infty} dt\, \sin\,(2\xi t)\mathrm{sh}(2t)\; K_0(2\xi\varepsilon\;\mathrm{ch}t),\ \text{see reference (5)}\right) .$$

The corresponding function

$$b(\xi,\varepsilon) = \int_{\varepsilon}^{\infty} B(\xi,\varepsilon') \frac{d\varepsilon'}{\varepsilon'} \tag{6}$$

$$(= -\frac{1}{2\xi} + \xi\varepsilon^2 \int_0^{\pi/2} d\theta e^{2\xi\theta} \sin(2\theta)\, K_o(2\xi\varepsilon \sin\theta) +$$

$$+ \xi\varepsilon^2 e^{\pi\xi} \int_0^{\infty} dt \cos(2\xi t) sh(2t)\, K_o(2\xi\varepsilon cht), \text{ see reference (5)})$$

has not been calculated.

II. Calculation of $A(\xi,\varepsilon)$ and $a(\xi,\varepsilon)$

These are both calculated at the same time in subroutine BIGA3(X,PP,A,CAPA) where $X = \xi\varepsilon$ and $PP \equiv \xi$.

(a) $\xi\varepsilon \leq 10^{-5}$,

$$A(\xi,\varepsilon) = 1 + \pi\xi$$
$$a(\xi,\varepsilon) = -\log(\xi\varepsilon) \tag{7}$$

(b) $10^{-5} < \xi\varepsilon < 4.0$

In this region interpolation in a smoothed table [subroutine INTERPA(POUT,XOUT,AOUT)] followed by conversion to A and a [in subroutine UNSCRAM(X,P,AOUT)] is used.

The Bessel functions to generate the A's were calculated from a program C3 NYU BES4 obtained from SHARE. This routine (called COMBES) computes the Bessel function $J_\nu(x)$ (with ν and x complex) for one argument and all orders by using the appropriate recursion relationships and normalization factors. $Y_\nu(x)$ is calculated by summation of $J_\nu(x)$. For details see reference 6.

The formulae relating A and a to the values obtained from the smoothed table in INTERPA are

$$A(\xi,\varepsilon) = (\xi\varepsilon)^2 e^{2\xi}\left[K_1^2(\xi\varepsilon)^2 + \left\{1 - \frac{\xi^2}{\varepsilon^2(\xi^2+1)}\right\} K_0^2(\xi\varepsilon)\right]\left\{\frac{\varepsilon^2-1}{\varepsilon^2} + \frac{1}{\varepsilon^2(\xi+1)}\right\}\cdot \mathrm{AOUT}(1)$$

$$a(\xi,\varepsilon) = (\xi\varepsilon)e^{2\xi}K_0(\xi\varepsilon)K_1(\xi\varepsilon)\cdot \mathrm{AOUT}(2) \quad . \tag{8}$$

(c) $\xi\varepsilon > 4.0$

In this region $e^{\pi\xi/2}K_{i\xi}(\xi\varepsilon)$ and $e^{\pi\xi/2}K'_{i\xi}(\xi\varepsilon)$ are calculated by SUBROUTINE KKP(X,P,CAY,CAYP) ($x \equiv \xi\varepsilon$, $P \equiv \xi$) by use of various asymptotic formulae:

(i) In the range $\xi^{2/3}(\varepsilon^2-1) \geq 0.01$

a formula due to Balogh is used:[7][8]

$$K_{i\nu}(\nu z) = \frac{\pi 2^{1/2}}{\nu^{1/3}} \exp\left(-\frac{\pi}{2}\nu\right)\left(\frac{\zeta}{z^2-1}\right)^{1/4}\left\{\mathrm{Ai}(\xi)\left[1+\sum_{s=1}^{m}\frac{A_s(\zeta)}{\nu^{2s}}\right] + \frac{\mathrm{Ai}'(\xi)}{\nu^{4/3}}\sum_{s=0}^{m-1}\frac{B_s(\zeta)}{\nu^{2s}}\right\} \tag{9}$$

where $\xi = \nu^{2/3}\zeta$, $\frac{2}{3}\zeta^{3/2} = (z^2-1)^{1/2} - \operatorname{arcsec} z$,

and the coefficients

$$A_s(\zeta) = \sum_{m=0}^{2s} (-1)^m b_m \zeta^{-3m/2} U_{2s-m}$$

$$\zeta^{1/2} B_s(\zeta) = \sum_{m=0}^{2s+1} (-1)^m a_n \zeta^{-3m/2} U_{2s-m+1}$$

$$a_o = 1, \quad a_s = \frac{(2s+1)(2s+3)\cdots(6s-1)}{s!(144)^s}$$

$$b_o = 1, \quad b_s = -\frac{6s+1}{6s-1} a_s$$

and $U_o = 1$

$$U_1 = \frac{v}{8}\left[\frac{5}{3} v^2 + 1\right]$$

$$U_2 = v^2\left[\frac{9}{128} + \frac{77}{192} v^2 + \frac{385}{1152} v^4\right]$$

$$U_3 = v^3\left[\frac{75}{1024} + \frac{4563}{5120} v^2 + \frac{17017}{9216} v^4 + \frac{85085}{82944} v^6\right]$$

$$U_4 = v^4 \frac{[4465125 + 94121676\, v^2 + 349922430\, v^4 + 446185740\, v^6 + 185910725\, v^8]}{39813120}$$

where $v = 1/(z^2-1)^{1/2}$

$$K_{i\nu}'(\nu z) = \frac{2^{1/2}\pi}{z} \exp\left(-\frac{\pi}{2}\nu\right)\left(\frac{\zeta}{z^2-1}\right)^{-1/4} \left\{ \frac{Ai(\xi)}{\nu^{4/3}} \sum_{s=0} \frac{C_s(\zeta)}{\nu^{2s}} + \frac{Ai'(\xi)}{\nu^{2/3}} \sum_{s=0} \frac{D_s(\zeta)}{\nu^{2s}} \right\} \quad (10)$$

where $$\zeta^{-1/2} C_s = \sum_{m=0}^{2s+1} (-1)^m b_m \zeta^{-3m/2} V_{2s-m+1}$$

$$D_s = \sum_{m=0}^{2s} (-1)^m a_m \zeta^{-3m/2} V_{2s-m}$$

and $V_1 = -\, v\,[\frac{3}{8} + \frac{7}{24} v^2]$

$$V_2 = -\, v^2[\frac{15}{128} + \frac{33}{64} v^2 + \frac{455}{1152} v^4]$$ (Notice: the negative sign was omitted in error in reference 7.)

$$V_3 = -\, v^3 \frac{[42525 + 451737\, v^2 + 883575\, v^4 + 475475\, v^6]}{414720} \quad .$$

The sums of terms involving the A,B,C and D coefficients are calculated in subroutine AB(LSWITCH,NU,ZETA,ZSQ,ACC,BCC,CVC,DVC). The subroutine is originally called with dummy variables so that data can be initialized (LSWITCH=1) Subsequent calls are with LSWITCH=2. Notice in particular that in the sums of terms multiplying the Airy functions there is considerable cancellation so Double-Precision is used. (There should be at least 16 digits accuracy.) The Airy Functions (calculated in AIRY) are obtained directly from tables given by Abramowitz and Stegun[9] (Table 10.11) which are stored as data, and then interpolated.

In the region $\xi\varepsilon \simeq 4.0$, comparison of $K_{i\xi}(\xi\varepsilon)$ with the COMBES routine gave accuracies of better than 5 significant figures, and the accuracy improves as $(\xi\varepsilon)$ increases. In fact, the Bessel functions were checked by direct numerical (Numerov) integration of the defining differential equation over an extended range including the region where the COMBES program was used.

(ii) In the range $\xi^{2/3}(\varepsilon^2-1) < 0.01$ a formula due to Erdelyi <u>et al</u>. is used[10]

$$K_{i\nu}(\nu z) = \frac{1}{3} \exp\left(\frac{-\pi\nu}{2}\right) \sum_{m=0} (-1)^m C_m \sin\,[(m+1)\pi/3]\; \Gamma\left(\frac{1}{3} m + \frac{1}{3}\right)\left(\frac{\nu z}{6}\right)^{-\frac{(m+1)}{3}} \qquad (11)$$

where $C_o = 1$ $\qquad C_1 = \nu(z-1)$

$$C_2 = \frac{C_1^2}{2} + \frac{1}{20} \qquad C_3 = \frac{C_1^3}{6} + \frac{C_1}{15}$$

$$C_4 = \frac{C_1^4}{24} + \frac{C_1^2}{24} + \frac{1}{280}$$

$$C_5 = \frac{C_1^5}{120} + \frac{C_1^3}{60} + \frac{43C_1}{4800}$$

and

$$K'_{i\nu}(\nu z) =$$

$$= \frac{1}{3}\exp\left(\frac{-\pi\nu}{2}\right)\sum_{m=0}(-1)^m \sin[(m+1)\tfrac{\pi}{3}]\Gamma(\tfrac{1}{3}m + \tfrac{1}{3})\left[C'_m\left(\frac{\nu z}{6}\right)^{-\frac{(m+1)}{3}} - \frac{(m+1)}{18}\, C_m\left(\frac{\nu z}{6}\right)^{-\frac{(m+4)}{3}}\right] \quad (12)$$

where $C'_o = C \qquad C'_1 = 1$

$$C'_2 = \nu(z-1)$$

$$C'_3 = \frac{1}{2}(C'_2)^2 + \frac{1}{15}$$

$$C'_4 = \frac{1}{6}(C'_2)^2 + \frac{1}{12}\, C'_2$$

$$C'_5 = \frac{1}{24}(C'_2)^4 + \frac{1}{20}\,(C'_2)^2 + \frac{43}{4800} \quad .$$

Accuracy is in excess of 4 figures even for $\varepsilon - 1$ less than 10^{-4}.

(d) If $\xi > 10 \Big/ \left[\sqrt{\varepsilon^2 - 1} - \cos^{-1}(1/\varepsilon)\right]$

then the following asymptotic form is appropriate

$$A(\xi,\varepsilon) = \pi\xi\sqrt{\varepsilon^2-1}\quad e^{-2\xi(\sqrt{\varepsilon^2-1} - \cos^{-1}(1/\varepsilon))}$$

$$a(\xi,\varepsilon) = \pi/2\ e^{-2\xi(\sqrt{\varepsilon^2-1} - \cos^{-1}(1/\varepsilon))} \quad . \qquad (13)$$

Notice that $\xi\sqrt{\varepsilon^2-1} = \rho\frac{\Delta E}{\hbar v} = z$ and for ε large (i.e., ρ large) the above formulae are just the asymptotic formulae for straight line paths (i.e., $A(z) = \pi|z|e^{-2|z|}$ and $a(z) = \pi/2\ e^{-2|z|}$) .

III. Calculation of $B(\xi,\varepsilon)$

The $B(\xi,\varepsilon)$ were calculated using the Hilbert transform of equation (4) with the $A(\xi,\varepsilon)$ functions obtained as in II. The interval $(0+,\infty)$ was transformed into (0+, ASYMVAL) where ASYMVAL is the value where the $A(\xi,\varepsilon)$ become less than 10^{-6}. The integrand in equation (4) has a discontinuity at $x = \xi$. The interval $(0,\xi)$ was thus divided into subintervals (usually 10) and integration in each sub-interval used a 10 point Gauss-Legendre routine. The interval (ξ,ASYMVAL) was then also divided into subintervals and 10 point Gauss-Legendre integration was used for subintervals of increasing x until the integral in the subinterval was less than 10^{-5} of the total integral. (For example, from ξ to 2ξ, we have steps of $0.25\,\xi$ with 10 point integration, and so on for (say) 4 steps between 2ξ and 10ξ, etc., until the convergence criterion is met.)

Notice that the integrand does not diverge as $x \to 0$ (for example, it tends to -2 as $\xi \to 0$ in this limit).

To test the accuracy of the above procedure the double integration for the imaginary part of equation (1) was performed numerically with the results shown:

ε	ξ	B(Hilbert Transform)	B(Double Integration)
1.4	5.0	1.849	1.846
1.05	50.0	3.081	3.099
1.01	10	-11.84	-11.89
1.01	0.5	-1.755	-1.737
1.01	0.1	-0.599	-0.558
1.0001	10.0	-13.41	-13.36
1.0001	1000.0	-282.00	-281.7
1.0001	30000.0	-2170.0	-2165.5

Satisfactory agreement is seen (better than or two percent), since it is not necessary to have the B's to too great accuracy.

For a given ε, $B(\xi,\varepsilon)$ was calculated for increasing ξ until it agreed (to 10^{-4}) with the following asymptotic expression(3)(5)

$$B(\xi,\varepsilon) \to \frac{\varepsilon^2}{2\xi(\varepsilon^2-1)^2}\left[(\pi-\cos^{-1}(1/\varepsilon))\,\frac{[2+\varepsilon^2]}{\sqrt{\varepsilon^2-1}}+3\right] \tag{14}$$

$$+\frac{\varepsilon^2}{2\xi^3(\varepsilon^2-1)^5}\left[\frac{(\pi-\cos^{-1}(1/\varepsilon))}{8\sqrt{\varepsilon^2-1}}\,(9\varepsilon^6+138\varepsilon^4+152\varepsilon^2+16)+\frac{1}{24}\,(229\varepsilon^4+592\varepsilon^2+124)\right].$$

Notice that for ε large this tends to $\pi/4\xi(\varepsilon^2-1)^{1/2}$ ($= \pi/4z$) which is the straight line result.

After $B(\xi,\varepsilon)$ was calculated and tabulated, the data were smoothed. The smoothed data are used in subroutine BFINAL. The smoothed values which are stored in the tables will here be referred to as ξ_T and B_T. Then:

(a)(i) $1.0001 \le \varepsilon < 1.3$

$$\xi = \left[\frac{\varepsilon^2}{(\varepsilon^2-1)^{3/2}}\right]\xi_T$$

$$B(\xi,\varepsilon) = \frac{\left[(\pi-\cos^{-1}(1/\varepsilon))\frac{[2+\varepsilon^2]}{\sqrt{\varepsilon^2-1}}+3\right]}{[(\pi/2)(\varepsilon^2-1)^{1/2}]}\;B_T(\xi_T,\varepsilon)\quad . \tag{15}$$

If $\xi_T > 12.5$ the asymptotic value of equation (14) is used. For $\xi_T \le 12.5$ interpolation in the table is used with linear interpolation in log $(1/(\varepsilon-1))$ for ε and quadratic interpolation for ξ_T.

(ii) $\varepsilon < 1.0001$

This is an unimportant region, and use of the value of $B_T(\xi_T,\varepsilon)$ at $\varepsilon = 1.0001$ is sufficient. Notice however, that when $\varepsilon = 1$, B diverges as $\xi\to\infty$ as $-\Gamma^2(2/3)\,\frac{6^{5/6}}{2^{3/2}}\,\xi^{2/3} = -2.88\,\xi^{2/3}$ (see reference 5).

(b) $1.3 \le \varepsilon \le 2.0$

No smoothing is used in this region and $B(\xi,\varepsilon)$ is stored directly. Quadratic interpolation in the ξ and ε directions are used. For $\xi > 30$ the asymptotic value of equation (14) is employed.

(c) $2.0 < \varepsilon \le \infty$

$$\xi = \frac{\left[(\pi-\cos^{-1}(1/\varepsilon))\frac{[2+\varepsilon^2]}{\sqrt{\varepsilon^2-1}} + 3\right]}{\left[\frac{\pi}{2}\frac{(\varepsilon^2-1)^3}{\varepsilon^4}\right]}\,\xi_T$$

$$B(\xi,\varepsilon) = \frac{\left[(\pi-\cos^{-1}(1/\varepsilon))\frac{(2+\varepsilon^2)}{\sqrt{\varepsilon^2-1}} + 3\right]}{\left[\frac{\pi(\varepsilon^2-1)^{3/2}}{4\varepsilon^2}\right]}\,B_2(\xi\sqrt{\varepsilon^2-1})\,B_T(\xi_T,\varepsilon) \tag{16}$$

The function $B_2(\xi\sqrt{\varepsilon^2-1})$ is the straight line B-function.[1]

If (i) $\xi_T < 0.0025$, we put $B(p,\varepsilon) = 0$

(ii) $0.0025 \le \xi_T \le 5.0$ and $\varepsilon < 100$, table interpolation in $B_T(\xi_T,\varepsilon)$ takes place with quadratic interpolation in the ξ_T direction and linear interpolation in $\log \varepsilon$ for ε. For $\varepsilon > 100$ in this range of ξ_T

$$B(\xi,\varepsilon) = B_2(\xi\sqrt{\varepsilon^2-1})$$

(iii) $\xi_T > 5.0$. The asymptotic value for $B(\xi,\varepsilon)$ of equation (14) is used.

In the important regions for the function $B(\xi,\varepsilon)$, ξ and ε are usually such that $B(\xi,\varepsilon)$ is positive. The regions of negative $B(\xi,\varepsilon)$ (see, for example, the figure in reference 11) is not very important. Also, when ε

gets small the asymptotic formula (equation (14)) is usually sufficient and for ξ small, ε is often sufficiently large that the straight line results are valid.

In the region of positive $B(\xi,\varepsilon)$ the accuracy should exceed 2%; in the negative region the accuracy is expected to decrease as $\xi \to 0$ and $\varepsilon \to 1$ (however, comparison with reference 5 shows good agreement even when $\varepsilon = 1.001$).

IV. Dipole Functions for a Repulsive Interaction

The functions $A_R(\xi,\varepsilon)$ and $a_R(\xi,\varepsilon)$ are very easily obtained from the attractive case,[3] since

$$A_R(\xi,\varepsilon) = e^{-2\pi\xi} A(\xi,\varepsilon)$$

and

$$a_R(\xi,\varepsilon) = e^{-2\pi\xi} a(\xi,\varepsilon) \quad .$$

The B function for the repulsive case has not been calculated, since inelastic collisions with ions are negligible and ξ is always very large. The asymptotic form is therefore sufficient, thus[3]

$$B_R(\xi,\varepsilon) = \frac{\varepsilon^2}{2\xi(\varepsilon^2-1)^2} \left[\frac{2+\varepsilon^2}{\sqrt{\varepsilon^2-1}} \cos^{-1}(1/\varepsilon) - 3 \right]$$

(notice: there is a typographical error in reference 3).
This result does not diverge as $\varepsilon \to 1$.

V. Quadrupole Broadening Functions

This section is included for the sake of completeness. It is found[1] that quadrupole terms are only important for levels which are essentially degenerate, thus we need only to evaluate the function corresponding to $A_4(z)$[1] in the limit of $\xi = 0$ (i.e., $\Delta E = 0$).

Thus, for an attractive potential[3]

$$\frac{A_4(\xi,\varepsilon)}{\rho^4} \equiv H(\varepsilon) = \frac{1}{a^4}\left\{\frac{1}{(\varepsilon^2-1)^2}\left[1+\frac{(\pi-\cos^{-1}(1/\varepsilon))}{(\varepsilon^2-1)^{1/2}}\right]^2+\frac{1}{3\varepsilon^4}\right\}$$

and

$$a_4(\xi,\varepsilon)\left(\frac{\Delta E}{hv}\right)^2 = h(\varepsilon) =$$

$$= \frac{1}{2a^2}\left[\frac{1}{2}\frac{(\pi-\cos^{-1}(1/\varepsilon))^2}{(\varepsilon^2-1)^2} - (\pi-\cos^{-1}(1/\varepsilon))\left(\frac{\pi}{2}-\cos^{-1}(1/\varepsilon)-\frac{1}{(\varepsilon^2-1)^{1/2}}-\frac{1}{(\varepsilon^2-1)^{3/2}}\right)\right.$$

$$\left.+\frac{1}{2(\varepsilon^2-1)}+\frac{1}{2}\left(\frac{\pi}{2}-\cos(1/\varepsilon)\right)^2+\frac{1}{3\varepsilon^2}\right] .$$

Notice that in the limit of ε large, both functions reduce to the straight line results (i.e., $A_4\ (0) = 4/3$ and $a_4 = \frac{2}{3}\left(\frac{\hbar v}{\rho\Delta E}\right)^2$) .

For the repulsive potential

$$H_R(\varepsilon) = \frac{1}{a^4}\left\{\frac{1}{(\varepsilon^2-1)^2}\left[1-\frac{\cos^{-1}(1/\varepsilon)}{(\varepsilon^2-1)^{1/2}}\right]^2+\frac{1}{3\varepsilon^4}\right\}$$

and

$$h_R(\varepsilon) = \frac{1}{2a^2}\left[\frac{1}{2}\frac{(\cos^{-1}(1/\varepsilon))^2}{(\varepsilon^2-1)^2}+\cos^{-1}(1/\varepsilon)\left(\frac{\pi}{2}-\cos^{-1}(1/\varepsilon)-\frac{1}{(\varepsilon^2-1)^{1/2}}-\frac{1}{(\varepsilon^2-1)^{3/2}}\right)\right.$$

$$\left.+\frac{1}{2(\varepsilon^2-1)}+\frac{1}{2}\left(\frac{\pi}{2}-\cos^{-1}(1/\varepsilon)\right)^2+\frac{1}{3\varepsilon^2}\right] .$$

Again these tend to the expected limit for ε large. The limit as $\varepsilon \to 1$ (i.e., as $\rho \to 0$) is more interesting. In particular,

$$h_R(\varepsilon\to 1) = \frac{1}{a^2}\left[\frac{\pi^2}{16}-\frac{1}{3}\right]$$

which is consistent with the $f_{E2}(0)$ function of Alder et al. (reference 4 pg. II.E 72).

Yet,

$$h(\varepsilon\to 1) \to \frac{\pi^2 a^2}{4\rho^2}$$

which diverges as $\rho \to 0$. This is a point worth noting, since Cooper and Oertel[12] used the relationship (2.38) of Biedenharn and Brussard,[13] which implies

$$f_{E2}(\xi)_{\text{Attractive}} = e^{2\pi|\xi|} f_{E2}(\xi)_{\text{Repulsive}} \quad .$$

Since the f_{E2} functions are equivalent to putting $\varepsilon = 1$, it is obvious that Biedenharn and Brussard's relation is in error for quadrupole interactions, although it holds for dipole interactions (i.e., $f_{E1\ \text{Attractive}} = e^{2\pi|\xi|} f_{E1\ \text{Repulsive}}$).

The reason that $f_{E1\ \text{Attractive}}$ does not diverge as $\rho \to 0$ is that the hyperbola is strongly curved, and the axial component of the electric field changes in direction during the collision and cancellation occurs. Whereas the quadrupole interaction (proportional to $\frac{1}{2}(3\cos^2\theta - 1)$) does not change sign and there is no cancellation to prevent divergence in the attractive case (as θ goes $\pi \to 0 \to -\pi$). There is no divergence in the repulsive case since the distance of closest approach is 2a.

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FORTRAN PROGRAMS FOR $a(\xi,\varepsilon)$, $A(\xi,\varepsilon)$, $B(\xi,\varepsilon)$

All page references in the following sub-programs are with respect to this report. If the input parameters to these routines are outside the intended range for this report, error messages will be printed, (for example, ε should be greater than unity).

Programs for $a(\xi,\varepsilon)$, $A(\xi,\varepsilon)$ are listed on pages 18 ff. (see page 17).

Programs for $B(\xi,\varepsilon)$ are listed on pages 34 ff. (see page 33).

$a(\xi,\varepsilon)$, $A(\xi,\varepsilon)$ are calculated by a FORTRAN sub program SUBROUTINE BIGA3.

For example:

CALL BIGA3(X,PP,A,CAPA)

where: $x = \xi\varepsilon$

$PP = \xi$

$A = a(\xi,\varepsilon)$

$CAPA = A(\xi,\varepsilon)$

SUBROUTINE BIGA3(X,PP,A,CAPA) **requires the following routines:**

```
      SUBROUTINE BIGA3(X,PP,A,CAPA)
C
C      10 - 25 - 1970
C
      DIMENSION AOUT(2)
      COMMON / SUB/ PI,HALFPI
      DATA(PI = 3.141592654),(UP=10.0)
      P = ABS (PP)
      EPSILON = X/P
      A = 0.0
      CAPA = 0.0
      IF(P .GT. X) RETURN
      IF(ABS (EPSILON-1.0) .LT.1.0E-50) GO TO 100
      ACOSINE = ACOS (1.0/EPSILON)
      ROOT = SQRT (EPSILON**2-1.0)
      ASYMVAL = UP / (ROOT - ACOSINE)
      IF(X .GT. 1.0E-5) GO TO 50
C
C     P * EPSILON LE 1.0E-5                        SEE PAGE 4, II (A)
C
   40 CAPA = 1.0 + PI * P
      A = - ALOG(X)
      RETURN
   50 IF(P .LT. ASYMVAL) GO TO 100
C
C     SEE PAGE 8, II (D)
C
      TEXP = EXP (-2.0*P * (ROOT - ACOSINE))
      CAPA = PI * P * ROOT * TEXP
      A = (PI/2.0) * TEXP
      RETURN
  100 IF(X.GT.4.0) GO TO 125
C
C     1.0E-5 LT P * EPSILON LE 4                   SEE PAGE 4, II(B)
C
      CALL INTERPA(P,X,AOUT)
      CALL UNSCRAM(X,P,AOUT)
      CAPA = AOUT(1)
      A = AOUT(2)
      RETURN
C
C     P * EPSILON GT 4                             SEE PAGE 5, II(C)
C
  125 CALL KKP(X,P,CAY,CAYP)
      XSQ = X**2
      COEF = 1.0
      CAPA = XSQ * COEF *(CAYP**2 + ((XSQ -  P**2)/XSQ) * CAY**2)
      A     = (-COEF) * X     * CAY * CAYP
      RETURN
      END
```

```
      SUBROUTINE INTERPA(POUT,XOUT,AOUT)
      DIMENSION A(29,29,2),AOUT(2),T(2,2),P(29),X(29)
      EQUIVALENCE(P,X)
      DATA((A(I),I=1,377)=
     * 1.02430, 28(0.0),
     * 1.01591,1.04513, 27(0.0),
     * 1.01609,1.03190,1.05892, 26(0.0),
     * 1.01686,1.02995,1.04483,1.06904,  25(0.0),
     * 1.01759,1.03041,1.04160,1.05544,1.07693, 24(0.0),
     * 1.01804,1.03129,1.04152,1.05150,1.06421,1.08321, 23(0.0),
     * 1.01844,1.03232,1.04262,1.05129,1.06029,1.07183,1.08862, 22(0.0),
     * 1.01879,1.03334,1.04412,1.05257,1.06010,1.06823,1.07865,1.09351,
     * 21(0.0),
     * 1.01908,1.03426,1.04569,1.05444,1.06159,1.06824,1.07557,1.08495,
     * 1.09810,   20(0.0),
     * 1.01933,1.03510,1.04722,1.05651,1.06382,1.06999,1.07589,1.08249,
     * 1.09091,1.10258, 19(0.0),
     * 1.02066,1.03996,1.05707,1.07213,1.08528,1.09665,1.10640,1.11467,
     * 1.12161,1.12736,1.15700,  18(0.0),
     * 1.02112,1.04189,1.06132,1.07945,1.09631,1.11192,1.12632,1.13957,
     * 1.15171,1.16277,1.22534,1.24052, 17(0.0),
     * 1.02131,1.04285,1.06351,1.08333,1.10227,1.12038,1.13764,1.15407,
     * 1.16966,1.18444,1.29128,1.33813,1.34792,  16(0.0))
      DATA( (A(I),I=378,580)=
     * 1.02139,1.04338,1.06480,1.08564,1.10591,1.12558,1.14467,1.16317,
     * 1.18107,1.19836,1.33921,1.42630,1.46751,1.46986,  15(0.0),
     * 1.02140,1.04368,1.06561,1.08713,1.10829,1.12904,1.14937,1.16929,
     * 1.18881,1.20788,1.37430,1.49617,1.57423,1.60869,1.59891,14(0.0),
     * 1.02140,1.04388,1.06615,1.08816,1.10995,1.13146,1.15270,1.17367,
     * 1.19434,1.21473,1.40075,1.55146,1.66349,1.73305,1.75649,1.73012,
     * 13(0.0),
     * 1.02136,1.04400,1.06652,1.08891,1.11112,1.13323,1.15516,1.17691,
     * 1.19847,1.21983,1.42125,1.59590,1.73797,1.84110,1.89899,1.90689,
     * 1.86049, 12(0.0),
     * 1.02131,1.04406,1.06679,1.08945,1.11205,1.13455,1.15702,1.17937,
     * 1.20164,1.22377,1.43756,1.63222,1.80065,1.93481,2.02644,2.06868,
     * 2.05718,1.98837, 11(0.0),
     * 1.02120,1.04410,1.06692,1.08986,1.11269,1.13558,1.15848,1.18132,
     * 1.20416,1.22690,1.45079,1.66240,1.85394,2.01643,2.14026,2.21674,
     * 2.23961,2.20571,2.11291, 10(0.0),
     * 1.02117,1.04406,1.06707,1.09012,1.11322,1.13645,1.15966,1.18285,
     * 1.20615,1.22942,1.46173,1.68781,1.89969,2.08797,2.24211,2.35209,
     * 2.40974,2.41009,2.35152,2.23381, 9(0.0))
      DATA( (A(I),I=581,725)=
     * 1.02105,1.04411,1.06716,1.09042,1.11371,1.13709,1.16052,1.18414,
     * 1.20777,1.23146,1.47089,1.70949,1.93937,2.15104,2.33355,2.47584,
     * 2.56824,2.60378,2.57901,2.49413,2.35102,  8(0.0),
     * 1.02094,1.04406,1.06722,1.09059,1.11399,1.13758,1.16132,1.18519,
     * 1.20915,1.23329,1.47866,1.72815,1.97409,2.20704,2.41595,2.58915,
     * 2.71579,2.78714,2.79768,2.74572,2.63333,2.46466,  7(0.0),
     * 1.02091,1.04401,1.06724,1.09066,1.11431,1.13802,1.16203,1.18615,
     * 1.21021,1.23460,1.48537,1.74442,2.00469,2.25706,2.49051,2.69309,
     * 2.85310,2.96041,3.00755,2.99064,2.90982,2.76910,2.57492, 6(0.0),
     * 1.02083,1.04411,1.06715,1.09083,1.11459,1.13856,1.16256,1.18669,
```

```
* 1.21134,1.23601,1.49111,1.75871,2.03181,2.30191,2.55825,2.78865,
* 2.98096,3.12392,3.20844,3.22855,3.18212,3.07112,2.90149,2.68203,
* 5(0.0),
* 1.02090,1.04378,1.06724,1.09104,1.11454,1.13890,1.16303,1.18758,
* 1.21196,1.23713,1.49615,1.77124,2.05602,2.34241,2.61993,2.87672,
* 3.10014,3.27818,3.40037,3.45893,3.44950,3.37175,3.22954,3.03065,
* 2.78622, 4(0.0))
 DATA( (A(I),I=726,841)=
* 1.02099,1.04371,1.06725,1.09068,1.11514,1.13909,1.16363,1.18793,
* 1.21296,1.23792,1.50071,1.78256,2.07778,2.37914,2.67645,2.95810,
* 3.21137,3.42368,3.58350,3.68142,3.71109,3.66989,3.55933,3.38507,
* 3.15673,2.88771, 3(0.0),
* 1.02057,1.04382,1.06761,1.09076,1.11500,1.13916,1.16393,1.18825,
* 1.21354,1.23878,1.50484,1.79252,2.09750,2.41269,2.72836,3.03342,
* 3.31535,3.56097,3.75807,3.89584,3.96617,3.96430,3.88937,3.74471,
* 3.53777,3.27990,2.98672,  2(0.0),
* 1.02129,1.04348,1.06793,1.09154,1.11553,1.13967,1.16498,1.18886,
* 1.21459,1.23967,1.50910,1.80229,2.11528,2.44294,2.77604,3.10333,
* 3.41255,3.69055,3.92435,4.10219,4.21429,4.25396,4.21808,4.10766,
* 3.92782,3.68770,3.40033,3.08343, 0.0,
* 1.01947,1.04329,1.06764,1.09038,1.11519,1.13990,1.16435,1.18840,
* 1.21504,1.23930,1.51168,1.80999,2.13168,2.47112,2.82010,3.16834,
* 3.50368,3.81294,4.08281,4.30056,4.45513,4.53806,4.54414,4.47206,
* 4.32459,4.10864,3.83497,3.51818,3.17802)
 DATA( (A(I),I=842,1218)=
* 1.01551, 28(0.0),
* 1.01816,1.03052,  27(0.0),
* 1.01928,1.03377,1.04236, 26(0.0),
* 1.01993,1.03578,1.04666,1.05235, 25(0.0),
* 1.02036,1.03718,1.04968,1.05769,1.06103, 24(0.0),
* 1.02060,1.03813,1.05187,1.06163,1.06725,1.06860, 23(0.0),
* 1.02077,1.03888,1.05360,1.06474,1.07217,1.07574,1.07538, 22(0.0),
* 1.02092,1.03949,1.05500,1.06727,1.07617,1.08158,1.08338,1.08150,
* 21(0.0),
* 1.02104,1.03999,1.05616,1.06938,1.07952,1.08644,1.09006,1.09028,
* 1.08706, 20(0.0),
* 1.02114,1.04042,1.05715,1.07117,1.08235,1.09058,1.09575,1.09776,
* 1.09658,1.09213, 19(0.0),
* 1.02164,1.04268,1.06241,1.08074,1.09758,1.11284,1.12645,1.13831,
* 1.14837,1.15655,1.12625,  18(0.0),
* 1.02181,1.04357,1.06456,1.08470,1.10392,1.12216,1.13935,1.15545,
* 1.17039,1.18410,1.24359,1.14468, 17(0.0),
* 1.02186,1.04401,1.06570,1.08686,1.10740,1.12731,1.14654,1.16502,
* 1.18270,1.19955,1.31223,1.30094,1.15601, 16(0.0))
 DATA( (A(I),I=1219,1421)=
* 1.02184,1.04428,1.06640,1.08821,1.10960,1.13057,1.15110,1.17110,
* 1.19056,1.20945,1.35741,1.40816,1.34222,1.16351,  15(0.0),
* 1.02184,1.04440,1.06689,1.08908,1.11109,1.13283,1.15425,1.17531,
* 1.19601,1.21630,1.38941,1.48627,1.48351,1.37362,1.16872, 14(0.0),
* 1.02178,1.04447,1.06713,1.08976,1.11219,1.13442,1.15651,1.17837,
* 1.20000,1.22136,1.41323,1.54568,1.59416,1.54474,1.39845,1.17245,
* 13(0.0),
* 1.02166,1.04449,1.06739,1.09018,1.11294,1.13561,1.15824,1.18076,
* 1.20301,1.22522,1.43171,1.59239,1.68307,1.68633,1.59580,1.41866,
```

```
     * 1.17519, 12(0.0),
     * 1.02166,1.04453,1.06754,1.09052,1.11364,1.13655,1.15957,1.18253,
     * 1.20539,1.22827,1.44641,1.63001,1.75601,1.80515,1.76629,1.63919,
     * 1.43546,1.17724, 11(0.0),
     * 1.02141,1.04453,1.06760,1.09073,1.11401,1.13724,1.16073,1.18405,
     * 1.20726,1.23061,1.45829,1.66103,1.81689,1.90618,1.91463,1.83659,
     * 1.67668,1.44971,1.17878, 10(0.0),
     * 1.02154,1.04466,1.06773,1.09101,1.11431,1.13781,1.16167,1.18500,
     * 1.20900,1.23277,1.46821,1.68691,1.86842,1.99298,2.04455,2.01356,
     * 1.89904,1.70948,1.46196,1.17995, 9(0.0))
      DATA( (A(I),I=1422,1566)=
     * 1.02143,1.04419,1.06799,1.09134,1.11470,1.13845,1.16238,1.18628,
     * 1.20998,1.23427,1.47670,1.70904,1.91258,2.06838,2.15919,2.17266,
     * 2.10360,1.95503,1.73848,1.47263,1.18084, 8(0.0),
     * 1.02177,1.04453,1.06771,1.09109,1.11448,1.13855,1.16303,1.18692,
     * 1.21161,1.23539,1.48371,1.72775,1.95107,2.13454,2.26100,2.31620,
     * 2.29174,2.18602,2.00561,1.76437,1.48201,1.18152, 7(0.0),
     * 1.02187,1.04362,1.06776,1.09111,1.11491,1.13893,1.16296,1.18799,
     * 1.21261,1.23668,1.48957,1.74435,1.98442,2.19275,2.35181,2.44624,
     * 2.46485,2.40272,2.26190,2.05163,1.78767,1.49034,1.18204,6(0.0),
     * 1.02162,1.04332,1.06811,1.09138,1.11511,1.13905,1.16301,1.18855,
     * 1.21363,1.23812,1.49560,1.75893,2.01412,2.24457,2.43343,2.56431,
     * 2.62444,2.60575,2.50661,2.33203,2.09374,1.80878,1.49779,1.18241,
     * 5(0.0),
     * 1.02124,1.04397,1.06652,1.09179,1.11637,1.14017,1.16308,1.18764,
     * 1.21348,1.23787,1.50034,1.77104,2.04050,2.29095,2.50707,2.67206,
     * 2.77175,2.79594,2.73962,2.60412,2.39718,2.13246,1.82803,1.50451,
     * 1.18269, 4(0.0))
      DATA( (A(I),I=1567,1682)=
     * 1.01929,1.04363,1.06923,1.09123,1.11424,1.13799,1.16626,1.19056,
     * 1.21491,1.23910,1.50470,1.78326,2.06401,2.33275,2.57374,2.77047,
     * 2.90807,2.97400,2.96105,2.86693,2.69585,2.45789,2.16823,1.84567,
     * 1.51059,1.18288,3(0.0),
     * 1.02469,1.04373,1.06682,1.09332,1.11610,1.14173,1.16362,1.18787,
     * 1.21402,1.24167,1.50610,1.79211,2.08525,2.37016,2.63485,2.86092,
     * 3.03431,3.14110,3.17124,3.12000,2.98824,2.78240,2.51467,2.20144,
     * 1.86191,1.51614,1.18301,  2(0.0),
     * 1.02591,1.04106,1.06408,1.09392,1.11979,1.14194,1.16971,1.19354,
     * 1.21370,1.23849,1.50943,1.80317,2.10493,2.40467,2.69049,2.94453,
     * 3.15189,3.29750,3.37061,3.36323,3.27330,3.10400,2.86430,2.56794,
     * 2.23234,1.87694,1.52122,1.18309,  0.0,
     * 1.01726,1.04364,1.06638,1.08573,1.11662,1.14342,1.16640,1.18582,
     * 1.21444,1.23900,1.51591,1.81069,2.11952,2.43593,2.74149,3.02169,
     * 3.26099,3.44460,3.55961,3.59674,3.55037,3.42113,3.21465,2.94187,
     * 2.61804,2.26124,1.89088,1.52590,1.18312)
      DATA(P=.02,.04,.06,.08,.1, .12,.14,.16,.18,.20,.4,.6,.8,1.0,1.20,
     1       1.40,1.60,1.80,2.0,2.20,2.40,2.60,2.80,3.0,3.20,3.40,3.60,
     2       3.80,4.00)
      M = N = 29
      DO 10 I = 1,M
      IF(POUT.LE.P(I)) GO TO 15
   10 CONTINUE
      GO TO 3000
   15 IP = I
```

```
      DO 20 I = 1,N
      IF(XOUT.LE.X(I)) GO TO 25
   20 CONTINUE
      GO TO 3000
   25 IX = I
      IF(IX.EQ. IP) GO  TO 200
      H = X(IX) - X(IX-1)
      PP = (XOUT-X(IX-1)) / H
C
C  IX .NE. IP
C
      IF(IP.GT.1) GO TO 100
C
C  IP = 1  0 .LE. P  .LE. .02  X(IX-1) .LE. X  .LE. X(IX)   4 PTS
C
      C = P(IP)
      QQ = POUT / C
      TEMPP = 1.0 - PP
      TEMPQ = 1.0 - QQ
      TA = TEMPP * TEMPQ
      TB = PP * TEMPQ
      TC = QQ * TEMPP
      TD = PP * QQ
C
C   F00 = 1.0    F10 = 1.0
C
      DO 30 I = 1,2
      AOUT(I) = TA + TB + TC*A(IP,IX-1,I) + TD*A(IP,IX,I)
   30 CONTINUE
      RETURN
C
C   REMAINDER OF TABLE  -  4 PTS.  -  NO PT. ON DIAGONAL
C
  100 C  = P(IP) - P(IP-1)
      QQ = (POUT-P(IP-1) ) / C
      TEMPP = 1.0 - PP
      TEMPQ = 1.0 - QQ
      TA = TEMPP * TEMPQ
      TB = PP * TEMPQ
      TC = QQ * TEMPP
      TD = PP * QQ
      DO 130 I = 1,2
      AOUT(I) = TA * A(IP-1,IX-1,I) + TB * A(IP-1,IX,I  + TC*A(IP,IX-1,I
     1) + TD * A(IP,IX,I)
  130 CONTINUE
      RETURN
C
C  IX = IP = 1  0  .LE.  X AND   P .LE. 0.02     3 PT
C
  200 IF(IX .NE. 1) GO TO 250
      QQ = POUT/.02
      PP = XOUT/.02
      TA = 1.0 - PP - QQ
      DO 210 I = 1,2
```

```
      AOUT(I) = TA + PP + QQ * A(IX,IP,I)
  210 CONTINUE
      RETURN
C
C  IX = IP
C
  250 H = X(IX) - X(IX-1)
      C = P(IP) - P(IP-1)
      PP = (XOUT-X(IX-1))/H
      QQ  = (POUT-P(IP-1)) / C
      TA = 1.0 - PP - QQ
      DO 270I = 1,2
      AOUT(I) = TA * A(IP-1,IX,I) + PP * A(IP-1,IX-1,I) + QQ * A(IP,IX,I
     1)
  270 CONTINUE
      RETURN
 3000 PRINT 650    ,POUT,XOUT,IP,IX
  650 FORMAT(* P,X*, 2F20.5,2I10)
      CALL EXIT
      END
```

```
      SUBROUTINE UNSCRAM (X,P,AT)
C
C     CONVERSION TO A, CAP A
C
      REAL K0,K1
      DIMENSION  AT(2)
      XSQ = X**2
      FK0 = K0( X)
      FK1 = K1(X)
      TEMP = EXP(2.0*P)
      EPSQ = XSQ/P**2
      UA = 1.0-P**2/((P**2+1.0)*EPSQ)
      EPSQ2 = EPSQ
      UB = (EPSQ2 - 1.0 + (1.0/(P    +1.0) ) ) / EPSQ2
      TCA = XSQ * TEMP * (FK1**2 + UA * FK0**2) * UB
      TA =    X     * TEMP * FK0 * FK1
      AT(1) = AT(1) * TCA
      AT(2 ) = AT(2) * TA
      RETURN
      END
```

```
      REAL FUNCTION K0(X)
      REAL I0
      K0 = 0.
      IF(X.LT.2.) GO TO 120
      X2 = 2./X
      K0 = 1./SQRT(X)*EXP(-X)*(1.25331414-.07832358*X2 +.02189568*X2**2
     2 -.01062446*X2**3+.00587872*X2**4-.0025154*X2**5+.00053208*X2**6)
      RETURN
  120 IF(X.LT.0.) RETURN
      T = X/3.75
      X2 = X/2.
      I0=1.+3.5156229*T**2+3.0899424*T**4+1.2067492*T**6+.2659732*T**8
     2  +.0360768*T**10 +.0045813*T**12
      K0=-ALOG(X2)*I0-.57721566+.4227842*X2**2+.2306976*X2**4+
     2 .0348859*X2**6+.00262698*X2**8+.0001075*X2**10+.0000074*X2**12
      RETURN
      END
      REAL FUNCTION K1(X)
      REAL I1
      K1 = 0.
      IF(X.LT.2.) GO TO 130
      X2 = 2./X
      K1 = 1./SQRT(X)*EXP(-X)*(1.25331414+.2349861*X2-.0365562*X2**2 +
     2 .01504268*X2**3-.00780353*X2**4+.00325614*X2**5-.00068245*X2**6)
      RETURN
  130 IF(X.LT.0.) RETURN
      T = X/3.75
      X2 = X/2.
      I1 = X*(.5+.87890594*T**2+.51498869*T**4+.15084934*T**6 +
     2 .02658733*T**8+.00301532*T**10+.00032411*T**12)
      K1 = I1*ALOG(X2)+1./X*(1.+.15443144*X2**2-.67278579*X2**4-
     2 .18156897*X2**6-.0191940*X2**8-.00110404*X2**10-.00004686*X2**12)
      RETURN
      END
```

```
      SUBROUTINE KKP(X,P,CAY,CAYP)
      COMMON /SUB/ PI,HALFPI
      DATA(KSWITCH=1)
      REAL K1,K0

C
C     K SUB I NU (NU Z)                              SEE PAGE 5, II(C)
C
      CAY = 0.0
      CAYP = 0.0
      IF(P .GT. 0.0000001) GO TO 200
      CAY = K0(X)
      CAYP = - K1(X)
      RETURN
  200 Z = X / P
      IF(Z .LT. 1.0) RETURN
      GO TO (250,350),KSWITCH

C     INITIALIZE AB  FOR KIDKI

  250 KSWITCH = 2
      CALL AB(1,DUM1,DUM2,DUM3,DUM4,DUM5,DUM6,DUM7)
  350 CALL KIDKI(P,Z,CAY,CAYP)
      RETURN
      END
```

```
      SUBROUTINE KIDKI(NU,Z,CAY,CAYP)
C
C     RETURNS EXP(PI Z/2) K AND K PRIME
C
      DIMENSION A(2),B(2),CV(2),DV(3)
      DIMENSION GAM(6),C(6),S(6),CP(6)
      COMMON /SUB/ PI,HALFPI
      REAL NU,NUSQ,NUFTH
      DOUBLE ZETA,TZET,U,ZSQ
      DATA(GAM = 2.6789385347,1.3541179394,1.0,0.8929795116,
     *           0.9027452929,1.0),
     *    (S = 0.866025403784,0.866025403784,0.0,-0.866025403784,
     *           -0.866025403784,0.0), (PI = 3.14159265359)
      DATA(HALFPI = 1.570796327)
      CONST = SQRT(2.0) * PI
      ZSQ = Z**2 - 1.0
      TWOTHD = 2.0/3.0
      IF( (NU**TWOTHD * ZSQ) .LT.0.01  )GO TO 200
C
C     BALOGH'S FORMULA                           SEE PAGE 5, II(C)
C
      NUSQ = NU**2
      NUFTH = NUSQ**2
      ONETHD = 1.0/3.0
      U = DSQRT(ZSQ)
      IF(Z .GT. 1.001) GO TO 10
      TZET = 0.0
      DO 50 I = 1,6
      II = 2 * I + 1
      TZET = TZET + (-1.0)**(I+1) * U**II/II
   50 CONTINUE
      GO TO 15
   10 YB = ACOS(1.0/Z)
      TZET = U - YB
   15 ZETA =    (1.5 * TZET) **TWOTHD
      XI = NU**TWOTHD * ZETA
   20 CALL AB(2,NU,ZETA,ZSQ,A,B,CV,DV)
      CALL AIRY(XI,AI,AIP)
      ATMP = A(2)
    2 IF(ABS (AI * A(1) + AIP * B(1)) .LE. ABS (AI) ) GO TO 1
      A(1) = B(1) = ATMP = B(2) = 0.0
      GO TO 5
    1 IF( ABS (AI*A(2) + AIP *B(2) ) .GT. ABS (AI * A(1) + AIP*B(1)) )
     .      ATMP = B(2) = 0.0
    5 TA = AI * (1.0 + A(1) + ATMP)
    6 TB = AIP * (B(1) + B(2))
    4 IF( ABS (AIP*DV(2) + AI * CV(1)) .LE. ABS (AIP*DV(1)) ) GO TO 3
      CV(1) = CV(2) = DV(2) = DV(3) = A(2) = 0.0
      GO TO 7
    3 IF(ABS (AIP*(DV(3)-A(2))+AI*CV(2)).GT.ABS (AIP*DV(2)+AI*CV(1)))
     .A(2) = CV(2) = DV(3) = 0.0
    7 TPA = AI *(CV(1) + CV(2))
    8 TPB = AIP * (DV(1) + DV(2) + (DV(3) - A(2) ))
      TPRE = CONST
```

```
      TMPRE= (ZETA/ZSQ)**0.25
      PRE = TPRE * TMPRE /  (NU**ONETHD)
      PREP = TPRE / (Z * (NU**TWOTHD) * TMPRE)
      CAY = PRE * (TA + TB)
      CAYP = PREP * ( TPA + TPB)
      RETURN
C
C     ERDELYI FORMULA                           SEE PAGE 7, II(C)
C
  200 EX = NU * (Z - 1.0)
      EX2 = EX**2
      EX3 = EX * EX2
      EX4 = EX2**2
      C(1) = 1.0
      C(2) = EX
      C(3) = 0.5 * EX2 + 0.05
      C(4) = (EX/3.0) * (0.5 * EX2 + 0.2)
      C(5) = (( (EX4 + EX2) / 6.0) + 1.0 / 70.0) * 0.25
      C(6) = (EX/60.0)* (0.5 * EX4 + EX2 + 43.0 / 80.0)
      CP(1) = 0.0
      CP(2) = 1.0
      CP(3) = EX
      CP(4) = 0.5 * EX2 + 1./15.
      CP(5) = (EX3/6.) + (EX/12.)
      CP(6) = (EX4/24.) + 0.05 * EX2 + 43./4800.
      SUM = 0.0
      SUMP = 0.0
      DO 300 MM = 1,6
      M = MM - 1
      TS = (-1.)**M * S(MM) * GAM(MM)
      TNUZ = NU*Z/6.
      TX = TNUZ **(-((M+1.)/3.))
      SUM = SUM + TS * TX * C(MM)
      SUMP = SUMP + TS *(CP(MM) * TX - ((M+1.)/18.)*C(MM)*TNUZ**(-((M+4.
     1)/3.)))
  300 CONTINUE
      CAY = SUM / 3.0
      CAYP = SUMP / 3.0
      RETURN
      END
```

```
      SUBROUTINE AB(LSWITCH,NU,ZETA,ZSQ,ACC,BCC,CVC,DVC)
C
C     SEE PAGE 7
C
      DIMENSION ACC(2),BCC(2),CVC(2),DVC(3)
      REAL NU
      DOUBLE A(5),B(5),AC(2),BC(2),DV(3),U(5),VV(12),D(12),ZT(12),VP(5),
     1        CV(2),NU13,NU23,DN,ZSQ,V,TEMPVP, TEMPCP, ZETA,
     2        V13, DD, ZNU, RCOEF, COEF, PRODA, PRODB, PRODC, DVP, DVV
      GO TO (100,200),LSWITCH
C
C     INITIALIZE A'S AND B'S
C
  100 A(1) = 1.0
      B(1) = 1.0
      DO 150 N = 2,5
      IS = N - 1
      DN = 1.0
      ME = 2 * IS
      DO 130 M = 1,ME
  130 DN = DN * (2.0 * IS + 2.0 * M - 1)
      A(N) = DN / (FACT(IS) * 144.0**IS)
      B(N) = -((6.0 * IS + 1.0) / (6.0 * IS - 1.0)) * A(N)
  150 CONTINUE
      RETURN
C
C     LSWITCH = 2
C
  200 IF(ZSQ .GT. 0.0) GO TO 201
      PRINT 600
  600 FORMAT(1H0,*AB ERROR  ZSQ = *,E20.9)
      CALL EXIT
  201 V = 1.0 / DSQRT(ZSQ)
      NU13 = NU**(1./3.)
      NU23 = NU**(2./3.)
      V13 = V / NU13
      DD = 39813120.
      ZNU = NU * ZETA**1.5
      RCOEF = ZNU**(1./3.)
      COEF = 1./RCOEF
      PRODA = 1.0
      PRODB = 1.0
      PRODC = 1.0
      DO 300 M = 1,12
      PRODA = PRODA * V13
      PRODB = PRODB * NU23
      PRODC = PRODC * ZNU
      VV(M) = PRODA
      D(M) = PRODB
      ZT(M) = PRODC
  300 CONTINUE
      U(1) = 1.0
      U(2) = (1./8.)* ((5./3.) * VV(3) + VV(1) /D(1))
      U(3) = ((9./128.) *VV(2) /D(2) +(77./192.) * VV(4) / D(1)
```

```
     *      + (385.0/1152.) * VV(6))
      U(4) = ((75./1024.) * VV(3) / D(3) + ( 4563./5120.) * VV(5)/D(2)
     *      + (17017./9216.) * VV(7) / D(1) + (85085./82944.) * VV(9))
      U(5) = ((4465125./DD) * VV(4) / D(4) + (94121676./DD) *VV(6)/D(3)
     *      + (349922430.0/DD) * VV(8) / D(2) + (446185740./DD) * VV(10)
     */D(1) + (185910725./DD) * VV(12) )
      DVP = 414720.
      VP(1) = 1.0
      VP(2) = -((3./8.) * VV(1)/D(1) +(7./24.) * VV(3))
      VP(3) = -((15./128.)*VV(2)/D(2) + (33./64.)*VV(4) / D(1)
     1          + (455./1152.)*VV(6))
      VP(4) = -((42525./DVP)*VV(3)/D(3) + (451737./DVP) *VV(5)/D(2)
     1          +(883575./DVP)*VV(7)/D(1) +(475475./DVP  )*VV(9))
      DVV = 39813120.
      VP(5) = -((5740875./DVV) * VV(4) / D(4) + (111234708./DVV) *
     1        VV(6) / D(3) + (396578754./DVV) * VV(8) / D(2) +
     2        (493152660./DVV) * VV(10) / D(1) + (202076875./DVV)
     3        * VV(12) )
      DV(1) = 1.0
      DO 450 J=2,3
      JJ = 2 * J - 1
      DV(J) = 0.0
      DO 400 I = 1,JJ
      II = JJ - I + 1
      TEMPVP = (-1.)**(I+1) * A(I) * VP(II)
      IF(I.GT.1) TEMPVP = TEMPVP/ZT(I-1)
  400 DV(J) = DV(J) + TEMPVP
  450 CONTINUE
      CV(1) = RCOEF * ( B(1) * VP(2) - B(2) * VP(1) / ZT(1))
      CV(2) = 0.0
      DO 475 J = 1,4
      JJ = 5 - J
      TEMPCP = (-1.)**(J-1) * B(J) * VP(JJ)
      IF(J .GT. 1) TEMPCP = TEMPCP / ZT(J-1)
  475 CV(2) = CV(2) + TEMPCP
      CV(2) = RCOEF * CV(2)
      AC(1) = B(1) *U(3) - B(2) * U(2) / ZT(1) + B(3) * U(1) /ZT(2)
      AC(2) = B(1) * U(5) - B(2) * U(4)/ZT(1) + B(3) * U(3) / ZT(2)
     *  - B(4) * U(2) / ZT(3) + B(5) * U(1) / ZT(4)
      BC(1) = COEF * (A(1) * U(2) - A(2) * U(1) / ZT(1))
      BC(2 ) = COEF *(A(1) * U(4) - A(2) * U(3) / ZT(1) + A(3) * U(2)
     *         / ZT(2) - A(4) * U(1) / ZT(3) )
      DO 485 LU = 1,2
      ACC(LU) = AC(LU)
      BCC(LU) = BC(LU)
      CVC(LU) = CV(LU)
      DVC(LU) = DV(LU)
  485 CONTINUE
      DVC(3) = DV(3)
      RETURN
      END
```

```
      SUBROUTINE AIRY (X,ERI,ERIP)
C
C     TABLES FROM ABRAMOWITZ AND STEGUN          SEE PAGE 7
C
      DIMENSION      AI(101,2),RZETA(21),FG(21,2),XX(101)
      DATA(XX = .00, .01, .02, .03, .04, .05, .06, .07, .08, .09,
     1          .10, .11, .12, .13, .14, .15, .16, .17, .18, .19,
     2          .20, .21, .22, .23, .24, .25, .26, .27, .28, .29,
     3          .30, .31, .32, .33, .34, .35, .36, .37, .38, .39,
     4          .40, .41, .42, .43, .44, .45, .46, .47, .48, .49,
     5          .50, .51, .52, .53, .54, .55, .56, .57, .58, .59,
     6          .60, .61, .62, .63, .64, .65, .66, .67, .68, .69,
     7          .70, .71, .72, .73, .74, .75, .76, .77, .78, .79,
     8          .80, .81, .82, .83, .84, .85, .86, .87, .88, .89,
     9          .90, .91, .92, .93, .94, .95, .96, .97, .98, .99, 1.0)
      DATA ((AI(I),I=1,95) =
     * 0.35502805, 0.35243992, 0.34985214, 0.34726505, 0.34467901,
     * 0.34209435, 0.33951139, 0.33693047, 0.33435191, 0.33177603,
     * 0.32920313, 0.32663352, 0.32406751, 0.32150538, 0.31894743,
     * 0.31639395, 0.31384521, 0.31130150, 0.30876307, 0.30623020,
     * 0.30370315, 0.30118218, 0.29866753, 0.29615945, 0.29365818,
     * 0.29116395, 0.28867701, 0.28619757, 0.28372586, 0.28126209,
     * 0.27880648, 0.27635923, 0.27392055, 0.27149064, 0.26906968,
     * 0.26665787, 0.26425540, 0.26186243, 0.25947916, 0.25710574,
     * 0.25474235, 0.25238916, 0.25004630, 0.24771395, 0.24539226,
     * 0.24308135, 0.24078139, 0.23849250, 0.23621482, 0.23394848,
     * 0.23169361, 0.22945031, 0.22721872, 0.22499894, 0.22279109,
     * 0.22059527, 0.21841158, 0.21624012, 0.21408099, 0.21193427,
     * 0.20980006, 0.20767844, 0.20556948, 0.20347327, 0.20138987,
     * 0.19931937, 0.19726182, 0.19521729, 0.19318584, 0.19116752,
     * 0.18916240, 0.18717052, 0.18519192, 0.18322666, 0.18127478,
     * 0.17933631, 0.17741128, 0.17549975, 0.17360172, 0.17171724,
     * 0.16984632, 0.16798899, 0.16614526, 0.16431516, 0.16249870,
     * 0.16069588, 0.15890673, 0.15713124, 0.15536942, 0.15362128,
     * 0.15188680, 0.15016600, 0.14845886, 0.14676538, 0.14508555)
      DATA ((AI(I),I=96,101) =
     * 0.14341935, 0.14176678, 0.14012782, 0.13850245, 0.13689066,
     * 0.13529242)
      DATA ((AI(I),  I=102,196) =
     * -0.25881940, -0.25880174, -0.25874909, -0.25866197, -0.25854090,
     * -0.25838640, -0.25819898, -0.25797916, -0.25772745, -0.25744437,
     * -0.25713042, -0.25678613, -0.25641200, -0.25600854, -0.25557625,
     * -0.25511565, -0.25462724, -0.25411151, -0.25356898, -0.25300013,
     * -0.25240547, -0.25178548, -0.25114067, -0.25047151, -0.24977850,
     * -0.24906211, -0.24832284, -0.24756115, -0.24677753, -0.24597244,
     * -0.24514636, -0.24429976, -0.24343309, -0.24254682, -0.24164140,
     * -0.24071730, -0.23977495, -0.23881481, -0.23783731, -0.23684291,
     * -0.23583203, -0.23480512, -0.23376259, -0.23270487, -0.23163239,
     * -0.23054556, -0.22944479, -0.22833050, -0.22720310, -0.22606297,
     * -0.22491053, -0.22374617, -0.22257027, -0.22138322, -0.22018541,
     * -0.21897720, -0.21775898, -0.21653112, -0.21529397, -0.21404790,
     * -0.21279326, -0.21153041, -0.21025970, -0.20898146, -0.20769605,
     * -0.20640378, -0.20510500, -0.20380004, -0.20248920, -0.20117281,
     * -0.19985119, -0.19852464, -0.19719347, -0.19585798, -0.19451846,
```

```
      * -0.19317521, -0.19182851, -0.19047865, -0.18912591, -0.18777055,
      * -0.18641286, -0.18505310, -0.18369153, -0.18232840, -0.18096398,
      * -0.17959851, -0.17823223, -0.17686539, -0.17549823, -0.17413097,
      * -0.17276384, -0.17139708, -0.17003090, -0.16866551, -0.16730113)
       DATA ((AI(I), I = 197,202) =
      * -0.16593797, -0.16457623, -0.16321611, -0.16185781, -0.16050153,
      * -0.15914744)
       DATA (RZETA = 1.5, 1.4, 1.3,1.2, 1.1, 1.0, 0.9, 0.8, 0.7, 0.6,
      *               0.5, 0.45, 0.4, 0.35, 0.3, 0.25, 0.2, 0.15, 0.1,
      *               0.05, 0.0)
       DATA (FG = 0.527027, 0.528783, 0.530601, 0.532488,0.534448,
      *           0.536489, 0.538618, 0.540844, 0.543180, 0.545636,
      *           0.548230, 0.549584, 0.550980, 0.552421, 0.553912,
      *           0.555456, 0.557058,0.558724, 0.560462, 0.562280,
      *           0.564190,
      *           0.619954, 0.617156, 0.614275, 0.611305, 0.608239,
      *           0.605068, 0.601782, 0.598372, 0.594823, 0.591120,
      *           0.587245, 0.585235, 0.583174, 0.581056, 0.578878,
      *           0.576635, 0.574320, 0.571927, 0.569448, 0.566873,
      *           0.564190)
       NXX = 101
       NRZ = 21
       IF(X .GE. 0.0) GO TO 100
       PRINT 600, X
   600 FORMAT(1H0,*AIRY  X = *,E20.9)
       CALL EXIT
   100 IF(X .GT. 1.0) GO TO 300
       DO 110 J = 1,NXX
       IF(X - XX(J)) 115,105,110
   105 ERI = AI(J,1)
       ERIP = AI(J,2)
       RETURN
   110 CONTINUE
   115 JSTART = J - 2
       IF(JSTART .EQ. 0) JSTART = 1
       IF(JSTART .EQ. (NXX-2)) JSTART = NXX - 3
       ERI = 0.0
       ERIP = 0.0
       DO 130 K = 1,4
       KK = K + JSTART - 1
       DN = 1.0
       DD = 1.0
       DO 120 J = 1,4
       IF(J .EQ. K ) GO TO 120
       JJ = J + JSTART - 1
       DN = DN * (X - XX(JJ))
       DD = DD * (XX(KK) - XX(JJ))
   120 CONTINUE
       TEMP = DN/DD
       ERI = ERI + TEMP * AI(KK,1)
       ERIP = ERIP + TEMP * AI(KK,2)
   130 CONTINUE
       RETURN
C
```

```
C       X .GT. 1.0
C
  300 ZETA = (2.0/3.0) * X**1.5
      RZET = 1.0/ZETA
      XFOURTH = X**0.25
      XPONE = 0.5 * EXP (-ZETA)
      DO 310 M = 1,NRZ
      IF(RZET - RZETA(M)) 310,305,315
  305 F = FG(M,1)
      G = FG(M,2)
      GO TO 350
  310 CONTINUE
  315 JSTART = M- 2
      IF(JSTART .EQ. 0) JSTART = 1
      IF(JSTART .EQ. (NRZ - 2)) JSTART = NRZ - 3
      F = 0.0
      G = 0.0
      DO 330 K = 1,4
      KK = K + JSTART - 1
      DN = 1.0
      DD = 1.0
      DO 320 J = 1,4
      IF(J .EQ. K) GO TO 320
      JJ = J + JSTART - 1
      DN = DN * (RZET - RZETA(JJ))
      DD = DD * (RZETA(KK) - RZETA(JJ))
  320 CONTINUE
      TEMP = DN / DD
      F = F + TEMP * FG(KK,1)
      G = G + TEMP * FG(KK,2)
  330 CONTINUE
  350 ERI = XPONE * F / XFOURTH
      ERIP = (-XPONE) * G * XFOURTH
      RETURN
      END
```

```
      FUNCTION FACT(N)
      TYPE DOUBLE FN
      IF(N) 100,101,102
  100 PRINT 300,N
  300 FORMAT(1H0,10X,*NEGATIVE FACTORIAL ARGUMENT*,I5)
      CALL EXIT
  101 FACT = 1.0
      RETURN
  102 FN = 1.0
      DO 105 I = 1,N
  105 FN = FN * I
      FACT = FN
      RETURN
      END
```

B(ξ,ε) is calculated by a FORTRAN sub-program

SUBROUTINE BFINAL.

a typical call to BFINAL would be:

CALL BFINAL (P,EPS,B)

where: P = ξ

EPS = ε

B = B(ξ,ε)

SUBROUTINE BFINAL requires the following routines:

FUNCTION BOFEP(E,P,PTEMP,K)	40
SUBROUTINE CONV(EPS,P)	41
SUBROUTINE K1K3(EPS,P,B,ZXI,YBXI,ISWITCH,K)	42
FUNCTION BASYM(E,P,K)	42
FUNCTION TERP(X,Y,XIN)	43
FUNCTION B2(Z)	43

```
      SUBROUTINE BFINAL(P,EPS,B)
      COMMON /TABLE/ EPSILON(15,3),PF(65,3),BF(65,15,3),NEPS(3),NEP(3),
     *          PLAST(3)
      DATA(NEPS=9,12,8),(NEP=65,43,38),(PLAST=12.5,30.0,5.0)
      DATA(EPSILON = 1.0001, 1.001, 1.01, 1.03, 1.05, 1.1, 1.2, 1.25,
     1               1.3, 6(0.0),  1.3, 1.35, 1.4, 1.45, 1.5, 1.55, 1.6,
     2               1.65, 1.7, 1.8, 1.9, 2.0, 3(0.0),  2.0, 3.0, 5.0,
     3               8.0, 10.0, 20.0, 50.0, 100.0,7(0.0) )
      DATA(PF = 0.0,0.02, 0.04, 0.06, 0.08, 0.1, .12, .14, .16, .18, .2,
     1          .4, .6, .8, 1.0, 1.2, 1.4, 1.6, 1.8, 2.0, 2.2, 2.4, 2.6,
     2          2.8, 3.0, 3.2, 3.4, 3.6, 3.8, 4.0, 4.2, 4.4, 4.6, 4.8,
     3          5.0, 5.2, 5.4, 5.6, 5.8, 6.0, 6.2, 6.4, 6.6, 6.8, 7.0,
     4          7.2, 7.4, 7.6, 7.8, 8.0, 8.2, 8.4, 8.6, 8.8, 9.0, 9.2,
     4          9.4, 9.6, 9.8, 10.0, 10.5, 11.0, 11.5, 12.0, 12.5,
     6          0.0, .02, .04, .06, .08, .1, .2, .3, .4, .5, .6, .7, .8,
     7          .9, 1.0, 1.5, 2.0, 2.5, 3.0, 3.5, 4.0, 4.5, 5.0, 5.5,
     8          6.0, 6.5, 7.0, 7.5, 8.0, 8.5, 9.0, 9.5, 10.0, 12.0, 14.,
     9          16.0, 18.0, 20.0, 22.0, 24.0, 26.0, 28.0, 30.0, 22(0.0),
     A          .0025, .005, .0075, .01, .02, .04, .06, .08, .1, .12,
     B          .14, .16, .18, .2, .4, .6, .8, 1.0, 1.2, 1.4, 1.6, 1.8,
     C          2.0, 2.2, 2.4, 2.6, 2.8, 3.0, 3.2, 3.4, 3.6, 3.8, 4.0,
     D          4.2, 4.4, 4.6, 4.8, 5.0, 27(0.0) )
C
C     SMOOTHED B-TABLE 1
C     1.0001 LE EPSILON LT 1.3                      SEE PAGE 10 (A)
C
      DATA ((BF(I),I=1,130)=
     *  0.00000,-.01705,-.03410,-.05115,-.06820,-.07641,-.08180,-.08719,
     *  -.09258,-.09643,-.09885,-.10620,-.09039,-.06446,-.03479,-.00440,
     *   .02487, .05211, .07669, .09842, .11734, .13292, .14572, .15396,
     *   .16220, .17044, .17847, .18001, .18155, .18309, .18462, .18335,
     *   .18132, .17929, .17726, .17439, .17082, .16725, .16368, .15999,
     *   .15602, .15205, .14808, .14412, .14032, .13652, .13272, .12892,
     *   .12545, .12206, .11867, .11528, .11217, .10925, .10634, .10342,
     *   .10066, .09819, .09573, .09327, .08775, .08259, .07821, .07406,
     *   .07042,
     *  0.00000,-.01658,-.03316,-.04974,-.06633,-.07678,-.08187,-.08696,
     *  -.09204,-.09694,-.09906,-.10605,-.09016,-.06439,-.03568,-.00743,
     *   .02082, .04907, .07658, .09368, .11079, .12789, .14500, .15587,
     *   .16258, .16930, .17602, .18190, .18234, .18279, .18323, .18367,
     *   .18206, .17941, .17677, .17412, .17125, .16744, .16363, .15983,
     *   .15602, .15211, .14816, .14420, .14025, .13639, .13275, .12912,
     *   .12548, .12185, .11860, .11545, .11229, .10914, .10615, .10349,
     *   .10084, .09818, .09552, .09325, .08771, .08271, .07812, .07413,
     *   .07031 )
      DATA((BF(I),I=131,260)=
     *  0.00000,-.03204,-.04764,-.06048,-.07022,-.07756,-.08370,-.08895,
     *  -.09334,-.09703,-.10009,-.10132,-.08867,-.06247,-.03269,-.00235,
     *   .02751, .05445, .07896, .10108, .12001, .13571, .14919, .16052,
     *   .16883, .17542, .18050, .18387, .18567, .18652, .18647, .18530,
     *   .18353, .18126, .17847, .17525, .17179, .16813, .16425, .16028,
     *   .15626, .15221, .14816, .14415, .14018, .13630, .13250, .12878,
     *   .12517, .12169, .11830, .11501, .11187, .10884, .10590, .10308,
     *   .10040, .09780, .09530, .09292, .08738, .08239, .07789, .07383,
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*    .07018,
*   0.00000,-.03243,-.04897,-.06121,-.07094,-.07839,-.08438,-.08948,
*   -.09378,-.09745,-.10046,-.10559,-.08752,-.06003,-.02889, .00259,
*    .03279, .06048, .08540, .10734, .12604, .14205, .15507, .16571,
*    .17363, .18006, .18491, .18755, .18914, .18973, .18913, .18769,
*    .18569, .18312, .17998, .17657, .17290, .16898, .16493, .16081,
*    .15663, .15245, .14829, .14416, .14013, .13617, .13229, .12853,
*    .12489, .12134, .11791, .11464, .11146, .10839, .10547, .10266,
*    .09995, .09736, .09489, .09250, .08696, .08201, .07755, .07353,
*    .06989 )
  DATA((BF(I),I=261,390)=
*   0.00000,-.03243,-.04886,-.06139,-.07105,-.07863,-.08475,-.08987,
*   -.09428,-.09783,-.10062,-.10459,-.08565,-.05695,-.02484, .00741,
*    .03797, .06613, .09122, .11257, .13122, .14754, .16003, .17029,
*    .17874, .18444, .18853, .19139, .19248, .19251, .19178, .19001,
*    .18762, .18479, .18143, .17775, .17386, .16975, .16553, .16125,
*    .15694, .15264, .14837, .14422, .14007, .13601, .13216, .12832,
*    .12458, .12110, .11762, .11427, .11116, .10806, .10508, .10234,
*    .09959, .09697, .09456, .09214, .08666, .08172, .07727, .07325,
*    .06962,
*   0.00000,-.03198,-.04914,-.06156,-.07139,-.07827,-.08509,-.08984,
*   -.09452,-.09758,-.10057,-.10242,-.08039,-.04901,-.01471, .01921,
*    .05116, .08014, .10541, .12730, .14588, .16105, .17213, .18282,
*    .18908, .19500, .19757, .19986, .19973, .19938, .19736, .19517,
*    .19188, .18846, .18419, .17992, .17564, .17132, .16669, .16206,
*    .15743, .15284, .14847, .14410, .13972, .13545, .13158, .12771,
*    .12384, .12010, .11679, .11347, .11016, .10699, .10420, .10141,
*    .09862, .09596, .09363, .09130, .08578, .08090, .07659, .07257,
*    .06910 )
  DATA( (BF(I),I=391,520)=
*   0.00000,-.03157,-.04887,-.06151,-.07131,-.07893,-.08503,-.09004,
*   -.09397,-.09702,-.09933,-.09600,-.06876,-.03258, .00592, .04296,
*    .07687, .10687, .13262, .15420, .17012, .18540, .19524, .20403,
*    .20880, .21265, .21368, .21394, .21234, .21015, .20680, .20302,
*    .19859, .19388, .18886, .18368, .17842, .17311, .16784, .16261,
*    .15764, .15285, .14806, .14327, .13848, .13413, .13018, .12623,
*    .12228, .11833, .11476, .11163, .10850, .10537, .10224, .09938,
*    .09692, .09447, .09202, .08956, .08438, .07954, .07539, .07153,
*    .06816,
*   0.00000,-.03161,-.04785,-.06105,-.07111,-.07845,-.08454,-.08952,
*   -.09336,-.09613,-.09824,-.09242,-.06211,-.02415, .01600, .05450,
*    .08909, .11954, .14520, .16656, .18363, .19698, .20691, .21274,
*    .21648, .22022, .22016, .21914, .21786, .21410, .21035, .20605,
*    .20093, .19581, .19035, .18474, .17914, .17357, .16801, .16254,
*    .15731, .15207, .14712, .14234, .13757, .13325, .12899, .12482,
*    .12106, .11729, .11391, .11091, .10791, .10491, .10191, .09891,
*    .09591, .09354, .09139, .08923, .08384, .07902, .07506, .07111,
*    .06782 )
  DATA( (BF(I),I= 521, 975)=
*   0.00000,-.03158,-.04792,-.06047,-.07027,-.07831,-.08394,-.08891,
*   -.09239,-.09511,-.09714,-.08722,-.05547,-.01525, .02599, .06573,
*    .10101, .13153, .15722, .17827, .19501, .20746, .21648, .22258,
*    .22618, .22766, .22726, .22420, .22114, .21808, .21354, .20822,
*    .20290, .19742, .19147, .18553, .17958, .17382, .16808, .16235,
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     *  .15689, .15173, .14657, .14147, .13701, .13254, .12808, .12408,
     *  .12028, .11648, .11286, .10966, .10646, .10326, .10052, .09782,
     *  .09513, .09265, .09038, .08811, .08332, .07899, .07467, .07068,
     *  .06766, 390(0.0) )
C
C     ACTUAL B-TABLE 2
C     1.3 LE EPSILON LE 2.0                          SEE PAGE 11, (B)
C
      DATA( (BF(I),I= 976,1105)=
     *    0.00000, -.16348, -.26064, -.33995, -.40848, -.46904, -.69532,
     *    -.84033, -.93753,-1.00021,-1.03685,-1.05300,-1.05263,-1.03870,
     *   -1.01358, -.77399, -.43202, -.05606,  .31451,  .67404, 1.00020,
     *    1.28943, 1.54059, 1.75435, 1.93254, 2.07771, 2.19280, 2.28089,
     *    2.34504, 2.38813, 2.41310, 2.42231, 2.41830, 2.30789, 2.11598,
     *    1.90148, 1.69468, 1.50860, 1.34756, 1.21059, 1.09511,  .99792,
     *     .91601 , 22(0.0),
     *    0.00000, -.16105, -.25564, -.33189, -.39700, -.45399, -.65836,
     *    -.77968, -.85118, -.88732, -.89736, -.88708, -.86093, -.82205,
     *    -.77294, -.43221, -.02425,  .38313,  .75521, 1.09165, 1.37352,
     *    1.60441, 1.78758, 1.92759, 2.02956, 2.09862, 2.13975, 2.15749,
     *    2.15594, 2.13895, 2.10943, 2.07035, 2.02387, 1.79949, 1.56531,
     *    1.35512, 1.17858, 1.03445,  .91808,  .82377,  .74682,  .68343,
     *     .63029 ,22(0.0) )
      DATA( (BF(I),I=1106,1235)=
     *    0.00000, -.15872, -.25074, -.32398, -.38579, -.43905, -.62235,
     *    -.72081, -.76764, -.77902, -.76442, -.73053, -.68170, -.62139,
     *    -.55225, -.13486,  .30988,  .71833, 1.06787, 1.35450, 1.57566,
     *    1.73830, 1.85000, 1.91871, 1.95267, 1.95875, 1.94304, 1.91075,
     *    1.86613, 1.81274, 1.75348, 1.69063, 1.62601, 1.37300, 1.15558,
     *     .98234,  .84786,  .74367,  .66203,  .59696,  .54407,  .50027,
     *     .46338,  22(0.0) ,
     *    0.00000, -.15637, -.24594, -.31621, -.37459, -.42437, -.58736,
     *    -.66323, -.68678, -.67518, -.63837, -.58337, -.51489, -.43656,
     *    -.35112,  .12068,  .57783,  .96502, 1.27087, 1.49834, 1.65372,
     *    1.74935, 1.79706, 1.80753, 1.78994, 1.75194, 1.69966, 1.63804,
     *    1.57098, 1.50112, 1.43085, 1.36155, 1.29436, 1.05739,  .87589,
     *     .74131,  .64100,  .56498,  .50562,  .45816,  .41934,  .38691,
     *     .35929, 22(0.0) )
      DATA( (BF(I),I=1236,1365)=
     *    0.00000, -.15414, -.24122, -.30852, -.36370, -.41001, -.55316,
     *    -.60728, -.60886, -.57583, -.51910, -.44552, -.36032, -.26719,
     *    -.16894,  .33761,  .78713, 1.13708, 1.38973, 1.55437, 1.64653,
     *    1.68219, 1.67687, 1.64256, 1.58875, 1.52276, 1.45006, 1.37468,
     *    1.29939, 1.22611, 1.15608, 1.09002, 1.02830,  .82494,  .68056,
     *     .57768,  .50230,  .44509,  .40021,  .36396,  .33401,  .30878,
     *     .28720, 22(0.0),
     *    0.00000, -.15203, -.23663, -.30105, -.35304, -.39576, -.51961,
     *    -.55285, -.53376, -.48120, -.40641, -.31683, -.21768, -.11275,
     *    -.00490,  .51924,  .94610, 1.24818, 1.44370, 1.54793, 1.58409,
     *    1.57217, 1.52811, 1.46400, 1.38877, 1.30869, 1.22810, 1.14985,
     *    1.07548, 1.00610,  .94206,  .88336,  .82993,  .66149,  .54718,
     *     .46707,  .40830,  .36335,  .32770,  .29868,  .27461,  .25415,
     *     .23659, 22(0.0) )
      DATA( (BF(I),I=1366,1495)=
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     *    0.00000, -.14985, -.23202, -.29354, -.34236, -.38089, -.48618,
     *    -.49960, -.46155, -.39108, -.30034, -.19706, -.08654,  .02738,
     *     .14194,  .66908, 1.06206, 1.30979, 1.44976, 1.49976, 1.48929,
     *    1.44050, 1.36941, 1.28717, 1.20130, 1.11666, 1.03615,  .96125,
     *     .89271,  .83058,  .77469,  .72453,  .67969,  .54224,  .45103,
     *     .38708,  .33983,  .30332,  .27415,  .25023,  .23027,  .21329,
     *     .19868, 22(0.0) ,
     *    0.00000, -.14775, -.22759, -.28618, -.33177, -.36797, -.45441,
     *    -.44853, -.39201, -.30540, -.20070, -.08593,  .03353,  .15393,
     *     .27257,  .79051, 1.14185, 1.33750, 1.42157, 1.42433, 1.37738,
     *    1.30266, 1.21504, 1.12405, 1.03549,  .95258,  .87680,  .80851,
     *     .74772,  .69383,  .64613,  .60401,  .56673,  .45424,  .38006,
     *     .32761,  .28853,  .25802,  .23350,  .21340,  .19648,  .18208,
     *     .16967, 22(0.0) )
      DATA( (BF(I),I=1496,1625)=
     *    0.00000, -.14577, -.22311, -.27896, -.32161, -.35447, -.42275,
     *    -.39868, -.32531, -.22399, -.10728,  .01687,  .14306,  .26762,
     *     .38807,  .88694, 1.19173, 1.33567, 1.37008, 1.33439, 1.26030,
     *    1.16880, 1.07279,  .97979,  .89363,  .81592,  .74708,  .68664,
     *     .63375,  .58763,  .54735,  .51204,  .48098,  .38780,  .32610,
     *     .28205,  .24894,  .22292,  .20195,  .18466,  .17010,  .15769,
     *     .14699, 22(0.0) ,
     *    0.00000, -.14175, -.21441, -.26461, -.30153, -.32711, -.36101,
     *    -.30308, -.20005, -.07401,  .06165,  .19890,  .33251,  .45958,
     *     .57784, 1.01654, 1.22277, 1.27257, 1.22903, 1.14049, 1.03587,
     *     .93134,  .83474,  .74917,  .67514,  .61181,  .55795,  .51212,
     *     .47296,  .43933,  .41027,  .38493,  .36271,  .29564,  .25033,
     *     .21746,  .19240,  .17258,  .15653,  .14323,  .13203,  .12246,
     *     .11422, 22(0.0) )
      DATA( (BF(I),I=1626,1950)=
     *    0.00000, -.13797, -.20598, -.25079, -.28178, -.30185, -.30256,
     *    -.21391, -.08514,  .05992,  .20816,  .35189,  .48656,  .60968,
     *     .71999, 1.08124, 1.19333, 1.16509, 1.07114,  .95643,  .84384,
     *     .74300,  .65677,  .58461,  .52475,  .47511,  .43381,  .39913,
     *     .36971,  .34451,  .32270,  .30365,  .28683,  .23551,  .20019,
     *     .17432,  .15442,  .13867,  .12585,  .11521,  .10623,  .09856,
     *     .09195, 22(0.0) ,
     *    0.00000, -.13667, -.19753, -.23765, -.26255, -.27642, -.24616,
     *    -.13011,  .01966,  .17869,  .33406,  .47877,  .60917,  .72370,
     *     .82198, 1.09767, 1.12793, 1.04340,  .92091,  .79832,  .69036,
     *     .60048,  .52749,  .46863,  .42100,  .38209,  .34994,  .32298,
     *     .30010,  .28040,  .26328,  .24824,  .23488,  .19370,  .16506,
     *     .14391,  .12760,  .11465,  .10409,  .09532,  .08793,  .08160,
     *     .07612, 217(0.0) )
C
C     SMOOTHED B-TABLE 3
C     2.0 GT EPSILON LE INFINITY                    SEE PAGE 11, (C)
C
      DATA( (BF(I),I=1951,2080)=
     *  -.97421,   -.68852,   -.58707,   -.49707,   -.28169,   -.12075,
     *  -.05982,   -.02569,   -.00017,    .02081,    .04057,    .05951,
     *   .07828,    .09760,    .30729,    .48640,    .57493,    .58957,
     *   .57587,    .55837,    .54506,    .53370,    .52582,    .52010,
     *   .51617,    .51324,    .51141,    .50958,    .50815,    .50714,
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*   .50613,   .50547,   .50486,   .50430,   .50387,   .50344,
*   .50312,   .50283,  27(0.0) ,
* -2.61045, -1.37569, -1.02995,  -.87639,  -.57477,  -.30191,
*  -.15183,  -.07734,  -.02930,   .00523,   .03119,   .05285,
*   .07121,   .08632,   .20854,   .31337,   .39987,   .46999,
*   .50859,   .54720,   .55318,   .55387,   .55145,   .54568,
*   .53981,   .53315,   .52648,   .52236,   .51922,   .51648,
*   .51450,   .51252,   .51112,   .50975,   .50864,   .50773,
*   .50688,   .50626,  27(0.0) )
  DATA( (BF(I),I=2081,2210)=
* -7.25985, -3.45485, -1.64059, -1.34423,  -.66897,  -.34955,
*  -.18538,  -.06638,   .00132,   .04141,   .07376,   .10610,
*   .12558,   .14254,   .24915,   .31181,   .36725,   .41363,
*   .44855,   .47569,   .50559,   .51503,   .52354,   .53369,
*   .53025,   .53039,   .52924,   .52442,   .52331,   .52033,
*   .51719,   .51574,   .51319,   .51151,   .51033,   .50871,
*   .50788,   .50703,  27(0.0) ,
*-10.39392, -4.19995, -2.58240, -1.95097,  -.72320,  -.26754,
*  -.09334,   .02079,   .08494,   .13020,   .16444,   .17916,
*   .19375,   .20833,   .30709,   .35538,   .39234,   .42172,
*   .44781,   .46999,   .47925,   .48858,   .50351,   .51236,
*   .50908,   .51178,   .52183,   .51642,   .51239,   .51401,
*   .51480,   .51039,   .50923,   .51144,   .50871,   .50634,
*   .50653,   .50672,  27(0.0) )
  DATA( (BF(I),I=2211,2340)=
*-12.22342, -4.75181, -2.27086, -1.77188,  -.63507,  -.21446,
*  -.04165,   .06149,   .10540,   .14931,   .19322,   .22335,
*   .23512,   .24688,   .33362,   .37564,   .40544,   .43029,
*   .45182,   .46992,   .48265,   .49159,   .50053,   .50947,
*   .51348,   .51474,   .51601,   .51728,   .51635,   .51507,
*   .51378,   .51250,   .51134,   .51018,   .50902,   .50795,
*   .50712,   .50629,  27(0.0) ,
*-17.18560, -4.93449, -2.51731, -1.70006,  -.54474,  -.06018,
*   .10521,   .21329,   .27134,   .29964,   .31983,   .3[illegible]686,
*   .34908,   .35471,   .40376,   .42789,   .44491,   .45837,
*   .46939,   .47894,   .48697,   .49128,   .48934,   .48967,
*   .49440,   .50561,   .50019,   .49603,   .49688,   .50334,
*   .50509,   .50011,   .49846,   .50036,   .50481,   .50104,
*   .49933,   .49990,  27(0.0 ) )
  DATA( (BF(I),I=2341,2925)=
*-11.38347, -4.45640, -2.80756, -1.40802,  -.36357,   .05302,
*   .22618,   .32724,   .39072,   .40166,   .41157,   .41995,
*   .42834,   .43319,   .45263,   .45965,   .47071,   .48885,
*   .49584,   .49502,   .49897,   .50159,   .49886,   .49355,
*   .49218,   .49272,   .49327,   .49381,   .49436,   .49490,
*   .49545,   .49600,   .49654,   .49707,   .49747,   .49787,
*   .49827,   .49867,  27(0.0),
* -6.06082, -3.14788, -1.76772, -1.14861,  -.25214,   .12786,
*   .26495,   .35971,   .44275,   .44560,   .45094,   .45623,
*   .46195,   .46602,   .47481,   .47974,   .48212,   .48230,
*   .47861,   .47598,   .48927,   .50561,   .51841,   .52185,
*   .52032,   .51590,   .51700,   .51391,   .50035,   .49271,
*   .49458,   .50436,   .50658,   .50119,   .49832,   .49866,
*   .50321,   .50407,  482(0.0) )
```

```
C
C     KK = TABLE NUMBER
C
  115 KK = 1
      IF(EPS .LT. 1.3) GO TO 120
      KK = 2
      IF(EPS.GT. 2.0) KK = 3
  120 IF(KK .NE. 2) CALL CONV(EPS,P)
      B = BOFEP(EPS,P,PTEMP,KK)
      RETURN
      END
```

```
      FUNCTION BOFEP(E,P,PTEMP,K)
C
C     INTERPOLATION IN THREE B-TABLES
C     K = TABLE NUMBER
C
      COMMON/TABLE/ EPSILON(15,3),PF(65,3),BF(65,15,3),NEPS(3),NEP(3),
     *             PLAST(3)
      DIMENSION ET(3)
      IQUAL = 1
      PTEMP = P
      IF(K.EQ. 2) GO TO 5
      CALL K1K3(E,P,DUM1,PTEMP,DUM2,1,K)
    5 IF(PTEMP .LE. PLAST(K) ) GO TO 10
      BOFEP = BASYM(E,P,K)
      RETURN
   10 IF(K.NE.3) GO TO 20
      IF(PTEMP .GE. 0.0025) GO TO 15
      BOFEP = 0.0
      RETURN
   15 IF(E .LE. 100.0) GO TO 20
      BOFEP = B2(P * SQRT (E**2 - 1.0) )
      RETURN
   20 NOE = NEPS(K)
      NOP = NEP(K)
      IF(E .GT. 1.0001) GO TO 25
      JEPS = 1
   23 IQUAL = 2
      GO TO 37
C     FIND EPSILON BOUNDS FOR INPUT E
   25 DO 30 J = 1,NOE
      JEPS = J
      IF(E - EPSILON(J,K) )35,23,30
   30 CONTINUE
   35 IF( (K.EQ.2) .AND. (NOE .EQ.JEPS) ) JEPS = JEPS - 1
C     FIND P BOUNDARIES FOR INPUT P
   37 DO 40 I = 1,NOP
      IP = I
      IF(PTEMP - PF(I,K) )50,45,40
   40 CONTINUE
   45 GO TO (48,46),IQUAL
   46 BTEMP = BF(IP,JEPS,K)
      IF(K .NE. 2) GO TO 200
      BOFEP = BTEMP
      RETURN
   48 ET(1) = BF(IP,JEPS-1,K)
      ET(2) = BF(IP,JEPS,K)
      IF(K .EQ. 2) ET(3) = BF(IP,JEPS+1,K)
      GO TO (90,72,100),K
   50 IF(NOP .EQ. IP) IP = IP - 1
      GO TO (60,55),IQUAL
   55 BTEMP = TERP(PF(IP-1,K),BF(IP-1,JEPS,K),PTEMP)
      IF(K .NE. 2) GO TO 200
      BOFEP = BTEMP
      RETURN
```

```
   60 GO TO (75,65,75),K
C     QUADRATIC INTERPOLATION IN P DIRECTION FOR K = 2
   65 DO 70 L = 1,3
      ET(L) = TERP(PF(IP-1,K),BF(IP-1,JEPS+L-2,K),PTEMP)
   70 CONTINUE
C     QUADRATIC INTERPOLATION IN EPSILON DIRECTION FOR K = 2
   72 BOFEP = TERP(EPSILON(JEPS-1,K),ET,E)
      RETURN
C     QUADRATIC INTERPOLATION IN PF DIRECTION FOR K = 1 OR 3
   75 DO 80 L = 1,2
      ET(L) = TERP(PF(IP-1,K),BF(IP-1,JEPS+L-2,K),PTEMP)
   80 CONTINUE
C     LINEAR INTERPOLATION IN EPSILON DIRECTION(LOG(1/(E-1)) FOR K = 1,
C                                               LOG(E) FOR K = 3)
      IF(K .EQ. 3) GO TO 100
   90 TEMP =ALOG (1.0/(EPSILON(JEPS-1,K)-1.0) )
      BTEMP = ET(1) + ((ALOG(1.0/(E-1.0) )- TEMP)/(ALOG(1.0/
     *        (EPSILON(JEPS,K)-1.0))- TEMP)) * (ET(2) - ET(1) )
      GO TO 200
  100 TEMP = ALOG(EPSILON(JEPS-1,K) )
      BTEMP = ET(1) + ((ALOG(E) - TEMP) / (ALOG(EPSILON(JEPS,K) ) - TEMP
     *) ) *   (ET(2) - ET(1) )
  200 CALL K1K3(E,P,BTEMP1,PTEMP,BTEMP,2,K)
      BOFEP = BTEMP1
      RETURN
      END
```

```
      SUBROUTINE CONV (EPS,P)
C
C     SETS UP CONVERSION FACTORS FOR TABLES 1 AND 2
C
      COMMON /COLD/ PI,EPSQ,SQUARE,ROOT,ACOSINE,PMC,TERMT
      DATA(PI = 3.141592654)
      EPSQ = EPS**2
      SQUARE = EPSQ - 1.0
      ROOT = SQRT (SQUARE)
      ACOSINE = ACOS (1.0/EPS)
      PMC = PI - ACOSINE
      TERMT = (PMC * ((2.0+EPSQ)/ROOT) + 3.0)
      RETURN
      END
```

```
      SUBROUTINE K1K3 (EPS,P,B,ZXI,YBXI,ISWITCH,K)
C
C     ISWITCH = 1 CONVERT P TO XI OR Z
C             = 2 CONVERT BXI OR Y TO B
C
      COMMON /COLD/ PI,EPSQ,SQUARE,ROOT,ACOSINE,PMC,TERMT
      IF(K .EQ. 3) GO TO 25
    5 COEF = PI * SQUARE**1.5 / (2.0* EPSQ)
      FNEW = EPSQ/ SQUARE
      GO TO (10,20),ISWITCH
   10 ZXI =    P * ROOT / FNEW
      RETURN
   20 B =YBXI * TERMT  / (COEF * FNEW)
      RETURN
   25 GO TO (30,40),ISWITCH
   30 TEMP = ROOT * (PI/2.0) * SQUARE**2.5 /(EPSQ**2* TERMT)
      ZXI = P * TEMP
      RETURN
   40 TEMP = (4.0*EPSQ*TERMT ) / (PI * SQUARE**1.5)
      B = YBXI * TEMP * B2(P * ROOT)
      RETURN
      END
```

```
      FUNCTION BASYM (E,P,K)
C
C     CALCULATES ASYMPTOTIC VALUE OF B(P,E) FOR P  GT P OF TABLES
C                                               SEE PAGE 11, (C)(II)
C
      COMMON /COLD/ PI,EPSQ,SQUARE,ROOT,ACOSINE,PMC,TERMT
      IF(K.EQ. 2) CALL CONV (E,P)
      TB = PMC/ (8.0*ROOT)
      TC = 9.0 *EPSQ**3 + 138.0 *EPSQ**2 + 152.0*EPSQ +16.0
      TD = (1.0/24.0)*(229.0*EPSQ**2+592.0*EPSQ+124.0)
      TA = EPSQ/(2.0*P**3 * SQUARE**5)
      TERM1 = (EPSQ/(2.0*P * SQUARE**2)) * TERMT
      TERM2 = TA * (TB * TC + TD)
      IF(TERM2 .GT. (1.0/3.0)*TERM1) TERM2 = 0.0
      BASYM = TERM1 + TERM2
      RETURN
      END
```

```
      FUNCTION TERP (X,Y,XIN)
C     QUADRATIC INTERPOLATION
      DIMENSION X(3),Y(3)
      SUM = 0.0
      DO 100 J = 1,3
      PROD   = 1.0
      DO 50 I  = 1,3
      IF(I .EQ. J) GO TO 50
      PROD = PROD * ((XIN-X(I) ) / (X(J) - X(I) ) )
   50 CONTINUE
      SUM = SUM + PROD * Y(J)
  100 CONTINUE
      TERP = SUM
      RETURN
      END
```

```
      FUNCTION B2(Z)
C
C                                                 SEE PAGE 11, (C) (II)
C
      DIMENSION ZZ(20),BB(20),N(5),C(5)
      DATA (ZZ = .0, .1, .2, .4, .6, .8, 1., 1.2, 1.4, 1.6, 1.8, 2., 3.,
     *          4., 5., 6., 7., 8., 9., 10.)   ,
     *     (BB = 0., 5.8501E-2, 1.6039E-1, 3.5887E-1, 4.9819E-1,
     *               5.7597E-1, 6.0588E-1, 6.0315E-1, 5.8021E-1,
     *               5.4590E-1, 5.0663E-1, 4.6692E-1, 3.0540E-1,
     *               2.1580E-1, 1.6640E-1, 1.3575E-1, 1.1509E-1,
     *               1.0005E-1, 8.8559E-2, 7.9470E-2)
      DATA(N=1,3,5,7,9),(C =  .7854,.8836,4.142,42.28,750.4)
      IF(Z .GT.10.0 ) GO TO 200
  100 DO 125 I = 1,20
      IF(Z - ZZ(I) ) 110,105,125
  105 B2 = BB(I)
      RETURN
  110 B2 = BB(I-1) + ((Z-ZZ(I-1))/(ZZ(I)-ZZ(I-1))) * (BB(I) - BB(I-1) )
      RETURN
  125 CONTINUE
  200 B2 = 0.0
      DO 225 I = 1,5
      B2 = B2 + C(I) / Z**N(I)
  225 CONTINUE
      RETURN
      END
```